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Crystal data (II) for some estrone-related c mp unds.*

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The lattice constants of eleven estrone-related compounds (Table 1) were determined on a General Electric XRD 5 X-ray diffraction unit equipped with a goniostat using Cu $K\alpha$ radiation. Space groups were established on the basis of systematic absences and optical activity.

All crystals were grown from solution. Flotation density measurements were used to calculate the number of molecules per unit cell. The high discrepancy between the measured (D_m) and calculated (D_x) densities of compound (3) is due to the crystallization of one molecule of ethanol per molecule of steroid. The density calculated taking the solvent of crystallization molecules into consideration is 1·151 g.cm^{-3} which agrees with the measured density. All of the other measured and calculated densities also agree within the experimental error (4·0%).

Compounds (1) and (2) each crystallized in two forms. Both of the (*a*) forms had similar but non-isomorphous unit cells. Compounds (2) and (3) are isomers but do not form isomorphous crystals.

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Table 1. *Crystal data* (II) *for some estrone-related compounds*

(1)(*a*), (*b*) 1,3,5(10)-Estratrien-3-ol-17-one
(2)(*a*), (*b*) 1,3,5(10)-Estratrien-3,17α-diol
(3) 1,3,5(10)-Estratrien-3,17β-diol
(4) 1,3,5(10)-Estratrien-3,17β-diol 3-methyl ether
(5) 1,3,5(10)-Estratrien-3,17β-diol 17-acetate
(6) 1,3,5(10)-Estratrien-17α-ethinyl-3,17β-diol 3-methyl ether
(7) 1,3,5(10)-Estratrien-3,17α-diol diacetate
(8) 1,3,5(10)-Estratrien-3-ol-17-one trimethyl acetate
(9) 1,3,5(10)-Estratrien-3,17α-diol 3-trimethyl acetate
(10) 1,3,5(10)-Estratrien-3,17β-diol dipropionate
(11) 1,3,5(10)-Estratrien-3,17β-diol 3-benzoate

	1(*a*)	1(*b*)	2(*a*)	2(*b*)	3	4	5
Formula	$C_{18}H_{22}O_2$	$C_{18}H_{22}O_2$	$C_{18}H_{24}O_2$	$C_{18}H_{24}O_2$	$C_{18}H_{24}O_2$	$C_{19}H_{26}O_2$	$C_{20}H_{26}O_3$
Mol. wt.	270·37	270·37	272·39	272·39	272·39	286·42	314·43
D_m (g.cm^{-3})	$1{\cdot}17_6$	$1{\cdot}24_8$	$1{\cdot}20_7$	$1{\cdot}20_7$	$1{\cdot}14_8$	$1{\cdot}20_6$	$1{\cdot}20_2$
D_x (g.cm^{-3})	1·220	1·249	1·190	1·190	0·985	1·186	1·220
Space group	$P2_1$	$P2_12_12_1$	$P2_1$	$C2$	$P2_12_12$	$P2_12_12$	$P22_12$
Z (calc.)	4	4	4	4	4	8	4
a (Å)†	9·297	10·051	9·127	19·212	12·241	14·004	13·803
b (Å)†	23·317	18·440	23·293	7·132	23·215	35·458	16·912
c (Å)†	7·662	7·755	7·238	13·422	6·466	6·470	7·331
β (°)	112·26	—	98·78	124·25	—	—	—
Volume (Å^3)	1471	1437	1521	1520	1837	3213	1711
Solvent	Methanol	Acetone	Methanol	Methanol	95% Ethanol	Heptane	95% Ethanol

† ±0·007.

Table 1 (*cont.*)

	6	7	8	9	10	11
Formula	$C_{21}H_{28}O_2$	$C_{22}H_{28}O_4$	$C_{23}H_{30}O_3$	$C_{23}H_{32}O_3$	$C_{24}H_{32}O_4$	$C_{25}H_{28}O_3$
Mol. wt.	310·44	356·47	354·49	356·51	384·52	376·50
D_m (g.cm^{-3})	$1{\cdot}22_2$	$1{\cdot}20_3$	$1{\cdot}16_8$	$1{\cdot}14_4$	$1{\cdot}20_9$	$1{\cdot}21_4$
D_x (g.cm^{-3})	1·217	1·246	1·175	1·153	1·182	1·251
Space group	$P2_1$	$P2_12_12_1$	$P2_1$	$P2_1$	$P2_1$	$P2_12_12_1$
Z (calc.)	4	4	2	2	4	4
a (Å)†	6·998	8·663	20·704	16·805	23·038	13·331
b (Å)†	39·737	29·390	7·318	9·714	9·057	23·846
c (Å)†	6·871	7·460	6·781	6·356	10·352	6·286
β (°)	117·58	—	102·51	98·36	95·36	—
Volume (Å^3)	1694	1899	1003	1027	2160	1998
Solvent	Heptane	Methanol	Propanol	Heptane–acetone	Acetone–methanol	95% Ethanol

† ±0·007.